Phase Behavior of Asymmetric Ionic Fluids

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The phase behavior of charge and size asymmetric electrolytes has been a topic of great interest because of its applications in colloidal and biophysical science. However a complete understanding of these systems remains lacking due to the difficulties that arise in theory and simulations. The phase transitions for 2:1 and 3:1 electrolytes obtained from detailed GCMC simulations have been reported in [1], but simulations of more highly charge asymmetric electrolytes become increasingly more challenging. We have adopted and adapted a reservoir GCMC method [2] to significantly improve the efficiency of the simulations allowing us to study systems with much higher charge asymmetry. The results we obtained are consistent with the critical points obtained by Linse in [3] for a 10:1 electrolyte with point counterions, but contradict the scaling law proposed in [4]. The simulation methods can also be easily extended to study systems of chain molecules, which will effectively model polyelectrolytes or ionic surfactants.

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